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Semiclassical quantization *via* the uncertainty principle

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Abstract : A semiclassical quantization procedure based on the quantum-mechanical uncertainty principle has been put forward. In cases, the scheme furnishes exact lower bounds to the eigenenergies; for others, approximate estimates are obtained. It is shown to obey the virial theorem, the Hellmann-Feynman theorem and a few exact scaling relations. Employing this strategy can treat both bound and resonant states. Relationship of the present endeavor with a semiempirical approach proposed recently for finding energy-eigenvalues of oscillators with quartic anharmonicity has also been established.

Keywords : Bound states, semiclassical quantization, uncertainty principle

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1. Introduction

In the course of his discussion on the zero-point energy, Schiff [1] provided a simple-minded route to estimate the ground-state energy of the harmonic oscillator (HO) *via* the uncertainty principle (UP), justifying that the former is a consequence of the UP. The procedure possesses basically a variational flavor yielding an approximate measure of the lowest energy of the HO. The purpose of the present communication is to *extend* such a view to encompass all possible energy-states and hence to sketch a route through which semiclassical quantization becomes possible, at least for simple systems. As we shall see, this UP-based scheme is much easier than the standard recipe based on the Wilson-Sommerfeld quantization rule. It is an integration-free technique. The associated physics of the problem remains also quite transparent. What is more, our scheme furnishes *lower bounds* to exact eigenenergies of bound states in quite a few cases, which, in the context of semiclassical methods, is admittedly a rare occurrence.

The organization will be as follows. First, in Section 2, we shall outline the scheme and point out how it is useful in furnishing true lower bounds to the exact energy eigenvalues in selected situations. Section 3 will be devoted to studies on a few of its salient features relating to properties of bound states and scaling; numerical estimates of energies in various situations will also be provided. In Section 4, we shall show how this strategy is able to handle the case of resonances. Its kinship with a successful semiempirical approach for studying the quartic anharmonic oscillator (AO) problem, proposed by Orland [2] and discussed in detail elsewhere [3] will concern us in Section 5. Finally, we reserve Section 6 for further remarks on this procedure.

2. The scheme

We start with a general result of the UP [4] which states that for some n-th eigenenergy state of a quantum system

$$\Delta x \Delta p \geq \left(n+\frac{1}{2}\right)\hbar \tag{1}$$

is true when potentials $V(x)$ have no infinite steps, with x in $]-\infty,\infty[$. It emerges from a constrained variation principle

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and the equality corresponds to eigenstates of the HO. Then, we employ the standard inequalities

$$\langle x^2\rangle \geq (\Delta x)^2, \quad \langle p^2\rangle \geq (\Delta p)^2. \tag{2}$$

Sometimes, depending on the nature of the potential $V(x)$, the semiclassical requirement

$$\langle x^m\rangle = \langle x\rangle^m \approx (\Delta x)^m \tag{3}$$

will also be assumed to hold. Here, by $\langle x\rangle$, we would mean $(\langle x^2\rangle)^{1/2}$ which is an approximation. But it is intuitively clear that the requirement is *not* undersirable because there is a possibility that bare $\langle x\rangle$ may have a vanishing magnitude dictated purely by symmetry of the Hamiltonian corresponding to the system.

To proceed, we consider the example of a quartic AO, with $V = x^2 + gx^4$, for demonstration. The energy E is given by

$$E = \langle T\rangle + \langle V\rangle = \langle p^2\rangle/2m + \langle x^2\rangle + g\langle x^4\rangle. \tag{4}$$

Now, by virtue of (1) and (2), it follows that

$$\langle T\rangle \geq \left[\left(n+\frac{1}{2}\right)\hbar\right]^2 / \left(2m(\Delta x)^2\right), \tag{5}$$

$$\langle V\rangle \geq (\Delta x)^2 + g\langle x^4\rangle \geq (\Delta x)^2 + g(\Delta x)^4, \tag{6}$$

where the last inequality in (6) follows from $\langle x^4\rangle \geq (\langle x^2\rangle)^2 \geq (\Delta x)^4$. Thus, one finally arrives at

$$E \geq E(\mathrm{UP}) = \left[\left(n+\frac{1}{2}\right)\hbar\right]^2 / \left(2m(\Delta x)^2\right) + (\Delta x)^2 + g(\Delta x)^4 \tag{7}$$

which is a neat inequality. We choose now Δx as a variational parameter [renamed as X later] in (7) and can optimize E. This will lead us to the required quantization. Note that in this case we get *lower bound* to the actual energy for *any state*. This is because, the inequality (7) is valid for any Δx. For other AO or for any problem involving not just x^2 and/or x^4 in the potential part, this nice bounding property may not hold. But, the kinetic energy part always obeys (5). One has to invoke approximation (3) to tackle $\langle V\rangle$. As a result, bounds to exact E are not obtained. For example, in case of the potential $V(x) = x^6$, one writes

$$E(\mathrm{UP}) = \left[\left(n+\frac{1}{2}\right)\hbar\right]^2 / \left(2m(\Delta x)^2\right) + (\Delta x)^6, \tag{8}$$

and hopes that $E \approx E(\mathrm{UP})$ will be satisfied because plainly $\langle x^6\rangle$ is approximated first by $(\langle x^2\rangle)^3$ and then (2) has been employed. Indeed, this will be the general strategy. Anyway, one may now continue with the $E(\mathrm{UP})$ expression above and, as before, optimize it to find $E_n(\mathrm{UP})$ that approximates E_n. Proceeding along similar lines, for $V(x) = x^8$, one will recover a similar equation for $E(\mathrm{UP})$ where $(\Delta x)^8$ will replace the last term in (8). A closer scrutiny however reveals that here the bounding property will be *regained*. The reason is the following series of inequalities :

$$\langle x^8\rangle \geq (\langle x^4\rangle)^2 \geq (\langle x^2\rangle)^4 \geq (\Delta x)^8. \tag{9}$$

It signifies that again $E \geq E(\mathrm{UP})$ in this case. Needless to mention, such an inequality will prevail for potentials like x^4, x^8, x^{16}, *etc.* and mixtures of such potentials including the harmonic one. The case of the pure HO is of special interest in the present context. We know that in this situation inequality (1) is an equality and (2) holds again with the equality sign, and hence $E = E(\mathrm{UP})$ is obeyed now so that extremisation will yield *exact* eigenvalues of energy.

It is now clear that the present strategy provides rough estimates of energy eigenvalues in general, as other semiclassical recipes do, but on certain special occasions we find here *lower bounds* to exact quantal eigenvalues which, to the best of our knowledge, are not obtainable through other techniques of comparable status.

3. Applications to bound states

Having discussed the general strategy, let us consider a few specific situations, analyze the general findings in detail and record some results. Henceforth, for convenience, we shall take $\hbar = 1$ and X will replace Δx.

3.1. Pure oscillators :

First, the case of pure oscillators, $V(x) = gx^{2N}$, will concern us. The energy expression then becomes

$$E(\mathrm{UP}) = \left[\left(n+\frac{1}{2}\right)\right]^2 / (2mX^2) + gX^{2N}. \tag{10}$$

The following observations are now important. (i) Optimization of X immediately shows that the virial theorem [5] $\langle T\rangle = N\langle V\rangle$ is valid here. (ii) The n-dependence of E follows easily on dimensional grounds. Letting $E \sim n^a$, [actually $(n + 1/2)^a$, but for large n this does not really matter] we get 'a' by separately insisting the same dependence for both the T and the V parts in (10). One finds

$$a = 2N/(1+N). \tag{11}$$

Table 1. Lower bound provided by E_n(UP) for $V(x) = gx^4$ [see (14)]

n	0	1	2	3	4	10
$g = 1$	0.7500	3.2451	6.4124	10.0429	14.0406	43 4531
	(1.0604)	(3.7997)	(7.4557)	(11.6447)	(16 2618)	(50.2563)
$g = 40000$	25.6496	110 9795	219.3013	343 4620	480.1806	1486.0735
	(36.2639)	(129.9470)	(254.9813)	(398.2447)	(556.1466)	(1718.7398)

Moreover, it can be verified here that $dE/dn = 2T/n$ is obeyed. Other ways [6] of arriving at such relations are not so simple. (iii) Similarly, the m-dependence follows. If $E \sim m^b$, we follow the same route to find that

$$b = -N/(N+1) \tag{12}$$

and $dE/dm = -T/m$, the content of the familiar Hellmann-Feynman theorem (HFT) [7] as discussed by Leung and Rosner [8]. It is worth mentioning that a Hamiltonian scaling argument yields the same result as (12). Defining

$$H(m) = -\nabla^2/2m + gx^{2N} \tag{13}$$

it follows that the relation $H(m) = m^b H$ (1) is exactly valid with b given by (12).

We shall now choose $m = \frac{1}{2}$ and demonstrate calculationally the workability of (10) after a due optimization. The final expression is

$$E_n(\mathrm{UP}) = (N+1)\left[g(n+1/2)^{2N}/N^N\right]^{1/(N+1)} \tag{14}$$

Table 1 displays results for the quartic oscillator case for various states n at two widely different values of g. Near-exact results [9], rounded at the fourth decimal place, are given everywhere in parentheses. The bounding nature of E_n(UP) is clearly seen. In Table 2, on the other hand, a comparison is

Table 2. Approximations to E_0 by E_0(UP) for $V(x) = x^{2N}$ [see (14)].

$N = 1$	$N = 2$	$N = 3$	$N = 4$
1.0000	0.7500	0.6204	0 5441
(1.0000)	(1.0604)	(1.1448)	(1.2258)

made among various ground state results at $g = 1$. Here we observe the following. (i) For $N = 1$, result is exact, as we previously commented. (ii) When N equals 2 or 4, one gets a lower bound, in accordance with our discussion in Section 2. Nevertheless, this bound is tighter in case of $N = 2$. The reason lies in the longer chain of inequalities involved in case of $N = 4$ that is apparent from (9). (iii) Even for $N = 3$, our result lies below the exact one. This is, however, purely accidental. One may appreciate that in this sextic oscillator case various inequalities like

$$\langle x^6\rangle \geq \left(\langle x^3\rangle\right)^2, \quad \langle x^4\rangle\langle x^2\rangle \geq (\Delta x)^6,$$
$$\langle x^4\rangle\langle x^2\rangle \geq \left(\langle x^3\rangle\right)^2 \tag{15}$$

are operative and it is difficult to say *a priori* which one is decisive at the final outcome based on the approximation $\langle x^6\rangle = (\Delta x)^6$ that has been made. (iv) Owing to the involvement of inequalities of varying degrees of tightness, the trend of E(UP) as a function of N does not agree with the exact one; little surprise is thus left on this point.

3.2. Mixed oscillators :

As our next attempt, we consider mixed AO of the general form

$$V(x) = \sum k_i x^i. \tag{16}$$

To insure the existence of bound states, one has to keep in mind that the summation in (16) should terminate at some even power of x. It is easy to see from the corresponding expression [like (8)] for E(UP), with $\hbar = 1$, $m = \frac{1}{2}$ and $\Delta x = X$, that the virial theorem is obeyed again after an extremization of X. Specifically, the determining equation for X_0, the optimum value of X, becomes

$$\sum i k_i X_0^{i+2} = 2(n+1/2)^2. \tag{17}$$

The optimum value of energy then becomes

$$E(\mathrm{UP}) = \sum (i/2+1) k_i X_0^i. \tag{18}$$

By employing (17) and (18), one obtains finally $\delta E/\delta k_j = X_0^j$, the HFT. In effect, this ensures proper *scaling* behavior of E with respect to $\{kj\}$. Such scaling

relations in the context of WKB approximation has been analyzed [10]; the relevance to quantum chemistry is also well known [11].

Having discussed the generalities, we now concentrate specifically on the potential $V(x) = x^2 + gx^4$ for which we have the bounding property of E(UP). From (18), one finds here

$$E(\mathrm{UP}) = 2Y + 3gY^2 \tag{19}$$

where $Y = X_0^2$ and the determining equation for Y is [see (17)]

$$\left(n+\tfrac{1}{2}\right)^2 / Y = Y + 2gY^2 \tag{20}$$

We now note the following. (i) When $g = 0$, $Y = (n+\frac{1}{2})$ and E(UP) provides exact result, as before. (ii) When $g \to \infty$, $Y \sim g^{1/3}$ and hence E(UP) will rise as $g^{1/3}$. The exact energy behaves in the same way. A Hamiltonian scaling argument again supports this observation. (iii) For small g, one can develop a perturbation series of E(UP) in g by employing (19) and (20). For brevity, we do not explicitly work it out here but like to remark that E_n(UP) is found to have a series expansion of the form

$$E_n(\mathrm{UP}) = 2(n+1/2) + g(n+1/2)^2 - g^2(n+1/2)^3 + \cdots \tag{21}$$

which may be compared with the exact one [12]

$$E_n = (2n+1) + 3g(2n^2+2n+1)/4 - g^2\left(17(2n+1)^3 + 67(2n+1)\right)/64 + \cdots \tag{22}$$

While the coefficients of the two expansions do not agree, and there is no reason to believe why they should, it is clear that the signs of correction terms follow the same pattern; particularly we note that the second order energy correction term is also *negative* in our case for *all* the states, like the actual finding. For large n, E_n/n possesses a power series in gn, as is true in our case as well.

Using (19) and (20), we may now check the lower bound property of E(UP). Table 3 displays a few results. Comparing them again with the near-exact results [9] given in the parentheses, one verifies the truth immediately. It is possibly of interest to notice another important numerical aspect in the present context. This concerns the real asymptotic behavior of E_n. In the large-g regime, $E_n(g)$ can be expanded as [13]

$$E_n(g) = g^{1/3}\left(\varepsilon_n + \alpha_n g^{-2/3} + \beta_n g^{-4/3} + \cdots\right). \tag{23}$$

One may here choose to evaluate ε_n approximately through the UP and examine its worth. It is defined by

$$\varepsilon_n = E_n/g^{1/3}, \quad g \to \infty, \tag{24}$$

and $E_n(\mathrm{UP})/g^{1/3}$ refers to our estimate. The required expression is easily obtained from (19) and (20):

$$\varepsilon_n = 3\left[(n+1/2)^2/2\right]^{2/3}. \tag{25}$$

Let us note that this estimate is actually the *same* as E_n(UP) given by (14), for $N = 2$, multiplied by $g^{-1/3}$. So, results for ε_n are indeed the values quoted in Table 1 at $g = 1$. The reason is obvious. When $g \to \infty$, the quartic AO considered here becomes virtually a pure quartic oscillator discussed previously and at $g = 1$ of the latter case the $g^{-1/3}$ factor becomes unity. The displayed results reveal that reasonable estimates are obtained on this count too. A comparison with the near-exact results [9,13] shown within parentheses in the same table justifies this conclusion. Except for the $n = 0$ state, the error is around 14%. This is tolerable in view of the extreme simplicity of the present scheme.

Table 3. Lower bound to exact energy by E_n(UP) for $V(x) = x^2 + gx^4$

n	0	1	2	3	4	10
$g = 1$	1.1823	4.2100	7.7971	11.7940	16.1247	47.1779
	(1.3924)	(4.6488)	(8.6550)	(13.1568)	(18.0576)	(53.4491)
$g = 40000$	25.6643	111.0100	219.3441	343.5155	480.2438	1486.1849
	(36.2745)	(129.9734)	(255.0177)	(398.2902)	(556.2005)	(1718.8344)

4. Applications to resonances

Quasi-eigenvalues in shape resonances have attracted considerable attention over the last few decades (see, *e.g.* [14]–[16] and references quoted therein). We wish to explore here how the present scheme works under such conditions. Again, let us choose the widely-employed potential $V(x) = x^2 + gx^4$, but this time with negative g. Then a local minimum around the origin will be supported by two symmetrically placed maxima at $x = \pm 1/(-2g)^{1/2}$ having a height of $-(4g)^{-1}$. Thus, although $V(x)$ does not strictly admit bound eigenstates, one can talk meaningfully about bound quasi-eigenstates if the lifetime of such states are long. These are resonant states.

We shall again use (19) and (20) to treat the above case. The relevant results are shown in Table 4. Here E refers to "exact" result [14] obtained by Drummond through Runge-Kutta integration and later corroborated by other workers.

Table 4. Properties of resonant states for $V(x) = x^2 + gx^4$ with negative g.

g	E	E(UP)	Y	$-(4g)^{-1}$
-0.05	0.9582	0.9872	0.513	5.0
-0.1	0.9007	0.9736	0.529	2.5
-0.2	0.7949	0.9436	0.569	1.25
-0.3	0.7475	0.9077	0 636	0.833
-0.4	0.7288	-	-	0 625
-0.5	0.7229	-	-	0.5
-0.6	0.7234	-	-	0.417
-1.0	0.7477	-	-	0.25

The following points are notable in this context. (i) Our results E(UP) are not close enough to E, even for small coupling strengths. A major reason is that we are dealing with states which satisfy the virial theorem exactly. But resonant states, conventionally found *via* the stabilization method [15] or else [14] *do not* obey this theorem. There is thus a qualitative difference between the states that we are considering here and those studied earlier and this is reflected in estimates for energy. (ii) In our case, the Y-values show a gradual increase with $-g$. It signifies the *optimum* spread in position. As the barrier height decreases with $-g$, delocalization is more favored; the rise is hence natural. (iii) Most important, no solution is found through E(UP) for large $-g$ values. It appears, however, that this is not entirely unreasonable. The last entry in the table lists also values of the barrier height. One hopes to find bound quasi-eigenstates only if the energy is *less* than this barrier height. This condition is clearly met for $-g$ somewhat below 0.4. So, the "exact" results do not seem to be physically [or semiclassically] quite meaningful. Indeed, there are three added complications. Published values [14] of lifetimes of these states show that, for example, the state at $g = -1.0$ is about 10^5 times more unstable than the same at $g = -0.05$. It is surprising whether the former state can still be called a quasi-eigenstate in the same spirit as the latter. There is no yardstick in this respect too in proper quantum domain. Another point is, one should choose states with small $\langle x^2 \rangle$ [Y in our case] as resonances [16]. But, we already noted that it increases rapidly with $-g$. An extrapolated value at $g = -1.0$ will surely be too large to be meaningful. The last hint is even more direct. Results reveal that E decreases first with $-g$, but then after a point [around $g = -0.5$] it increases. This behaviour is not in accord with a transparent physics of the problem. We are hence compelled to disregard at least those E values beyond $g = -0.5$ or so as genuine resonant state energies. In that case, however, performance of E(UP) is not unreasonable, particularly in providing a *limit* of g up to which a resonant state may exist.

The above discussion will certainly be more illuminating if we consider (20), the determining equation for Y. Figure 1 shows the relevant part of the $Y - g$ plot. For

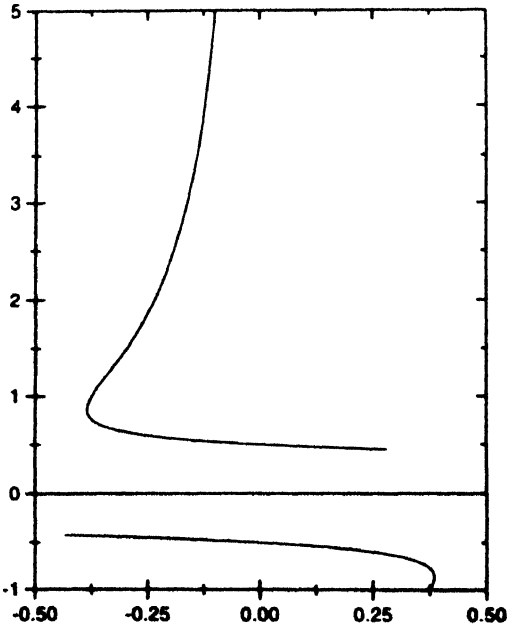

Figure 1. Plot of Y [see (20)] as a function of the coupling strength g, showing the limit of applicability in the negative-g regime in the UP-based scheme.

$g > 0$, only one positive, and hence acceptable, solution of Y exists. The situation is very transparent. On the other hand, there are two positive solutions of Y for $g < 0$, up to

$g \approx -0.385$. Of these, the lower positive root, having continuity with the $g = 0$ solution, should concern us. Gradually, however, the higher root tends towards the lower one as $-g$ increases. They finally become degenerate at $g \approx -0.385$ with $Y \approx 0.86$. But, there is no *acceptable* solution of Y for $-g > 0.385$. A limit is thus clearly put in respect of resonances by this recipe on the coupling strength. That something more subtle should happen in region beyond that permitted by UP is at the same time obvious.

5. Semiempiricism

The quartic AO that we have been concentrating on so far has been treated in various ways. We now like to sketch a semiempirical strategy [2] in successfully tackling this problem. Here, one demands a solution of energy that satisfies (i) the virial theorem, (ii) the HFT and (iii) the semiclassical condition $\langle F^m(x)\rangle = \langle F(x)\rangle^m$. Using these three conditions, one arrives (see, *e.g.* ref. [3] for a detailed account) at a nonlinear differential equation, solves it and fits the integration constant to reproduce the exact $E(g)$ at some chosen g ; the solution is subsequently used to obtain energies at neighboring g-values with good accuracy. The method is thus essentially semiempirical in nature. The working scheme is summarized as follows, with two parameters A and B, the former possessing the status of an integration constant :

$$E = 3AB + (2B)^{-1}; \tag{26}$$

$$g = AB^3 - B/2. \tag{27}$$

From these equations, one finds

$$EB^2 - 3g - 2B = 0. \tag{28}$$

The scheme now is to first put a known E at a specific g in (28) to estimate B. Then, use is made of (27) to find A at that g value. Once A is obtained, the problem is solved. One can now employ this A value in (27) at some other g to get B and then put the new B value in (26) to get E at this altered g. Orland [2] used a known value of E at $g = 100$.

It is of interest to check how this strategy works if we supply the E value at $g = 0$, for this is an exactly known result. Putting accordingly $E = 1$, $g = 0$ in (28), we obtain $B = 0$ [neglected] or $B = 2$. Using (27), we find $A = 1/8$. Finally, one sees that (26) and (27) take respectively the forms

$$E = 3B/8 + (2B)^{-1}; \tag{29}$$

$$g = B^3/8 - B/2. \tag{30}$$

One may now see how this pair of equations works in describing resonant states. To this end, we refer to Figure 2 which shows possible values of B at a given g value, positive or negative. We find that there is one positive value of B for $g > 0$. But, if $g < 0$, there are two positive values of B. While it is not immediately apparent from the discussion here that we have to stick only to positive B values, our UP-based scheme says so. Let us compare these last two equations with (19) and (20) taking $n = 0$, as we are considering ground state. It is remarkable that the equations are equivalent if we associate B with $1/Y$. In other words, we now have a clear *physics* for B. It is the inverse of $\langle x^2\rangle$. Clarly then, it cannot be negative. So, finally we can disregard the negative solutions for B. Figure 2 then shows that resonant states

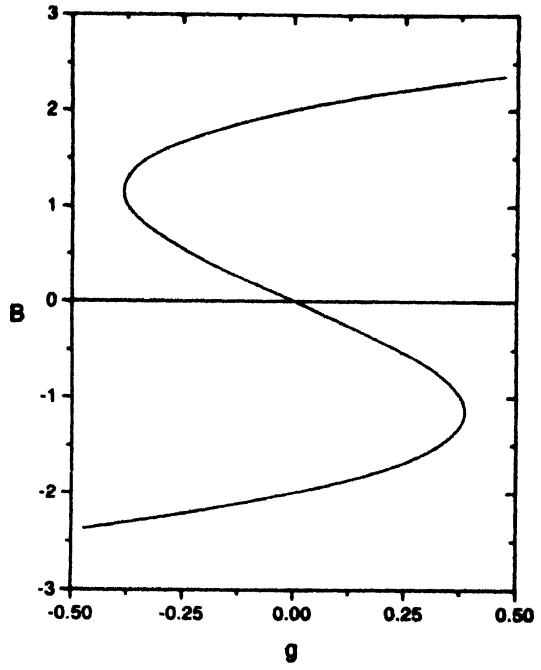

Figure 2. Plot of B [see (30)] as a function of the coupling strength g, showing the limit of applicability in the negative-g regime in Orland's semiempirical strategy.

cannot be supported beyond $g = -0.385$. Additionally, we now have a ready interpretation of the semiempirical strategy that is said to work for other potentials as well.

6. Conclusion

To summarize, here we have found a semiclassical quantization scheme by virtue of the general UP that works under various circumstances and offers us a clear physics. On some occasions, lower bounds to exact quantal results are found and reasons behind it explained. Along with bound states, resonant states can also be treated by

this recipe. The extension to multidimensional problems may be useful.

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